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14. ABSTRACT
The general objective of this project was to develop a new algorithmic capability to be employed in the next generation of relaistic non-sterilized simulation, which could be schieved at three to four orders of magnitude more efficiently than Monte-Carlo simulations.

(See attached)

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FINAL REPORT:
AN ADAPTIVE RANDOM DOMAIN DECOMPOSITION METHOD FOR STOCHASTIC CFD AND MHD PROBLEMS
AFOSR GRANT NUMBER: FA9550-06-1-0148

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Abstract

The PI and his students were the first to conduct uncertainty quantification work sponsored by the Computtaional Mathematics program of AFOSR and developed the generalized polynomial chaos (gPC) approach that has had great impact in CFD and in other application areas. In the current project we developed the theoretical foundations for effective *adaptive* formulations to model uncertainty in large-scale simulations involving fluid dynamics (CFD) and magneto-hydro-dynamics (MHD) applications. The basic idea is to decompose the multi-dimensional random space into small elements within which gPC expansions are employed. Both Galerkin and collocation projections - including sparse grids – have been employed in our formulation. The work completed includes large-scale simulations but also theoretical advances on the bounds for convergence rates, as well as new variance-based sensitivity analysis for MHD problems.

Objectives

The general objective of this project was to develop a new algorithmic capability to be employed in the next generation of realistic **non-sterilized** simulation, which could be achieved at three to four orders of magnitude more efficiently than Monte-Carlo simulations. The *specific* objective was to develop an adaptive stochastic simulation in multi-dimensional random space for systems of conservation laws that govern CFD and MHD problems.

Approach

Generalized polynomial chaos (gPC) or Wiener-Askey expansions is a method developed by the PI and his students with partial AFOSR support almost ten years go. This method is similar to spectral techniques - but in high-dimensions - so both Galerkin and collocation projections can be employed to produce the algebraic equations from the partial differential equations. Recently, we developed a more robust method using the multi-element approach. We have formulated both a Galerkin approach, the multi-element generalized polynomial chaos (ME-gPC), as well a collocation approach, the multi-element probabilistic collocation method (ME-PCM). Both methods converge very fast, with the error in *mean* and in *variance* decaying as

$$\text{ME-gPC:} \quad \epsilon \propto N^{-2(p+1)} \qquad \text{or} \qquad \text{ME-PCM:} \quad \epsilon \propto N^{-2N_c},$$

where N is the number of random elements per dimension, p is the order of the polynomial chaos, and N_c is the number of collocation points per random direction.

At the heart of this method is the ability to represent effectively arbitrary probability measures. To this end, we developed an efficient procedure in constructing orthogonal polynomials "on-the-fly" that can be used as trial bases in each random subdomain. This construction is based on the *correspondence principle* between orthogonality weights and probability measures, which we established in the previous AFOSR grant. The two new multi-element methods (ME-gPC or ME-PCM) are conceptually similar to the spectral/*hp* element method for deterministic problems, i.e., convergence is achieved by either increasing the number of random elements or the degree of the generalized polynomial chaos expansion. They provide robustness and controlled high-order accuracy in problems requiring long-time integration or involving stochastic discontinuities, e.g. transitional flows.

Main Results

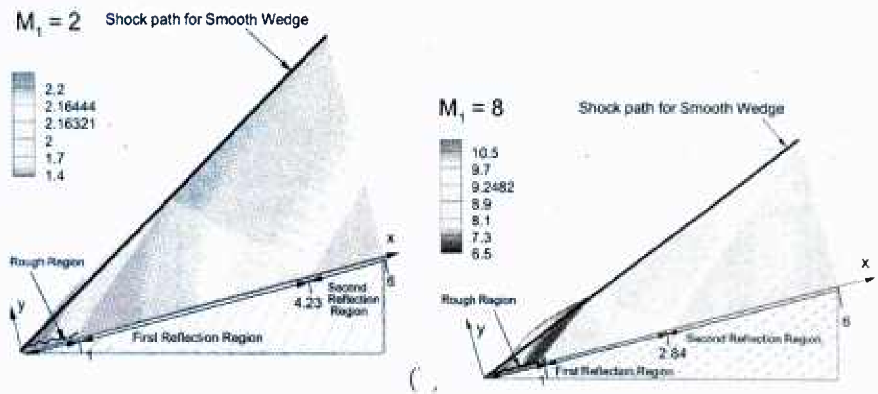
The main algorithmic result of this project is the resolution of the Gibbs phenomenon in parametric space using the multi-element approach. This is encountered when bifurcations take place as a result of increasing a certain parameter. Combined with heuristic and rigorous adaptive criteria – wherever possible – this leads to a very efficient and effective solution of the problem. We have also completed the theoretical foundation of ME-PCM, demonstrating convergence rates under different norms, see (Foo et al, 2008). In addition, we have developed a new variance-based sensitivity analysis and we applied it to stochastic models for two-fluid MHD as well as supersonic plasma flow past a cylinder (Lin & Karniadakis, 2008). We highlight some of the simulations results next.

Stochastic CFD Simulations

Next, we present results for our study past a rough wedge, for details see (Lin et al, PRL, 2007). We consider the following conditions: The semi-infinite wedge, see Fig. 1, is truncated after $x = 6$ while the rough region is $x \in [0, 1]$ (x is normalized by the roughness length d); the angle of the unperturbed shock is $\chi_0 = 45°$ and the angle of the wedge is $\theta_0 = 14.7436°$. We consider two values of the inflow Mach number, i.e., $M_1 = 2$ and $M_1 = 8$. All the physical quantities can be obtained from the Rankine-Hugoniot relations, hence the outflow boundary conditions can be set up accurately. In the simulations, we employ a fifth-order weighted essentially non-oscillatory scheme for spatial discretization with 1000×1000 grid points in the domain $[0, 6] \times [0, 4]$. The stochastic simulations are based on a probabilistic collocation method and multi-dimensional integration using sparse grids to deal with many dimensions (up to 12).

Typical pressure contours corresponding to one realization for $M_1 = 2$ and $M_1 = 8$ are presented in Fig. 1. A reflection of Mach waves at the wedge surface is observed in both cases, with the reflection point for $M_1 = 8$ being closer to the wedge apex than for the $M_1 = 2$ case.

Next, we present results for the *mean* of the perturbed normalized lift force for $M_1 = 2$ and $M_1 = 8$, respectively, in Figs. 2(a) and (b) as a function of the distance from the wedge apex, for roughness amplitude $\epsilon = 0.003$ and $\epsilon = 0.1$, and correlation length $\frac{A}{d} = 0.1$ and $\frac{A}{d} = 1$. For roughness amplitude $\epsilon = 0.003$, the numerical results based on the full solution of the stochastic nonlinear Euler equations agree well with the second-order stochastic perturbation solutions (denoted as "Analytical Soln" in the plot), thus verifying the ϵ^2 dependence. However, for roughness amplitude $\epsilon = 0.1$, the numerical solution deviates significantly from the theory, leading to a scaling $\propto \epsilon^c$ with $1 < c < 2$. There seems to be a qualitative flow change for large roughness height as well, with the perturbed lift force being almost constant beyond the roughness region. This can be explained by the significant distortion of



(a) (

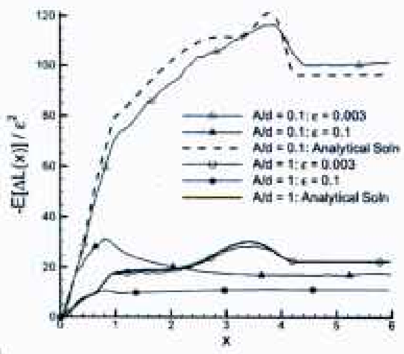
Figure 1: (in color) Flow structure (flow is from left to right): Pressure contours (one realization) for (a), $M_1 = 2$ and (b), $M_1 = 8$ (the pressure contours for $M_1 = 8$ are stretched 4 times perpendicular to the wedge surface for visualization purposes). ($\epsilon = 0.01$ and $A/d = 0.1$).

the characteristic lines that lead to a large variation of the location of the reflection point on the wedge for different realizations. This, in turn, will result in an *averaging out* effect in the mean solution with no discernible reflection region anymore. The enhanced lift force generated due to roughness can be significant and of the same order of magnitude as the lift of the base flow (smooth wedge). Moreover, within the rough region strictly positive mean lift forces are observed for both $M_1 = 2$ and $M_1 = 8$ cases and are increasing significantly both with respect to Mach number and also with d/A; the latter implies that a large lift force can be obtained for *fine* granularity roughness. For large roughness (large ϵ) the perturbed lift increases almost monotonically with the distance to the apex but large variations occur, especially for $M_1 = 8$, beyond the roughness region for small ϵ.

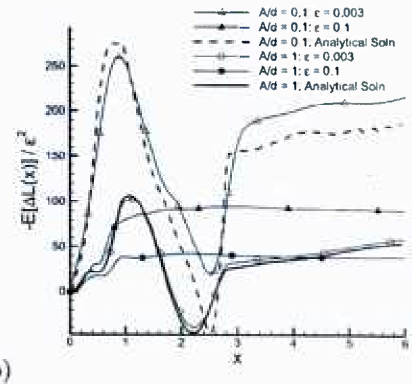
Stochastic MHD Simulations

We study parametric uncertainties involved in plasma flows and apply stochastic sensitivity analysis to rank the importance of all inputs. Specifically, we employ different gradient-based sensitivity methods, namely Morris, sparse probabilistic collocation, Quasi-Monte Carlo, and Monte Carlo. These methods go beyond the standard "One-At-a-Time" sensitivity analysis and provide a measure of the nonlinear interaction effects for the uncertain inputs. The objective is to perform systematic stochastic simulations of plasma flows treating only as *stochastic processes* the inputs with the highest sensitivity index, hence reducing substantially the computational cost. Two plasma flow examples are presented to demonstrate the capability and efficiency of the stochastic sensitivity analysis. The first one is a two-fluid model in a shock tube while the second one is a one-fluid/two-temperature model in flow past a cylinder.

To demonstrate the capability and study the convergence of these sensitivity algorithms, we systematically test the parametric sensitivity and interaction of a function with three random input parameters. The test function with three random input parameters is: $d_3 = 63e^{4x_1} - 70e^{3x_2} + 15e^{2x_3}$. Fig. 3 demonstrates the convergence of mean and standard deviation of d_3 obtained by Morris method, Monte Carlo method and collocation method on sparse grids. Fast convergence of both mean and standard deviation solution obtained by collocation method on sparse grids is observed for small number of



(a)



(b)

Figure 2: Enhanced lift force: Distribution of the perturbed mean lift along the wedge surface (the wedge apex is at $x = 0$). (**a**) $M_1 = 2$ and (**b**) $M_1 = 8$. (The lift is normalized by $P_2\,d$ where P_2 is the pressure after the shock of the corresponding smooth wedge.)

random inputs, compared to Morris and Monte Carlo method. Morris method has similar convergence rate as Monte Carlo method. Thus, for small number of random inputs, the collocation method on sparse grids is a better choice. However, when the number of random inputs increases the efficiency of collocation method on sparse grids decreases substantially. For very large number of random inputs, the Morris method and the Monte Carlo method will be more efficient than the collocation method.

In single-fluid/two-temperature plasma flow simulation, there are mainly five uncertainty sources, i.e., Re_i, Re_e, Pr_i, Pr_e and Re_{mag}. We consider as a benchmark example the supersonic flow $Ma = 2$ past a cylinder. To efficiently capture the primary uncertainty source from the above five random inputs, sensitivity analysis is performed. Figure 4 presents the statistics of the streamwise velocity for the ion Reynolds number Re_i described as a random process. A complete analysis is given in (Lin & Karniadakis, 2008/2009).

Acknowledgement/Disclaimer

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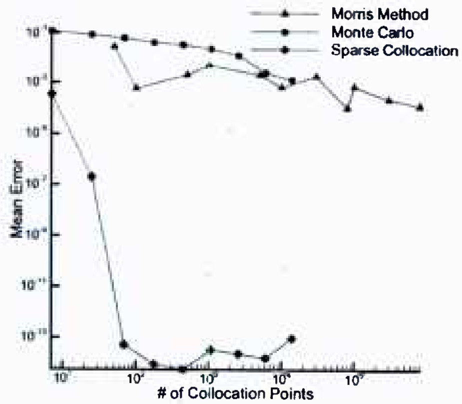
Personnel Supported During Duration of Grant

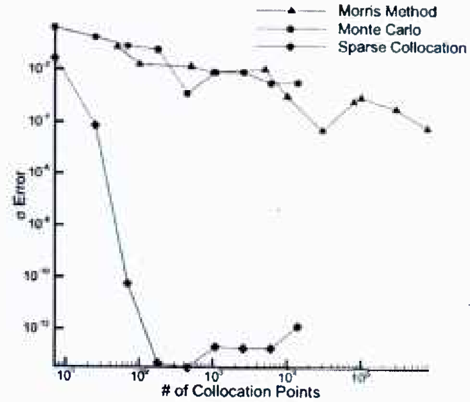
- Faculty: G.E. Karniadakis, Professor of Applied Mathematics, Brown University.
- Faculty: C.-H. Su, Professor of Applied Mathematics, Brown University.
- PhD Students: Xiaoliang Wan, Guang Lin, Xian Luo, Brown University.
- Visitor: Dr Daniele Venturi, University of Bologna, Italy.

Honors & Awards

- US Association of Computational Mechanics, 2007 Computational Fluid Dynamics award.



(a)



(b)

Figure 3: Convergence of mean and standard deviation of d_3 obtained by different sensitivity algorithms.

- Associate Fellow of the American Institute of Aeronautics and Astronautics (AIAA), 2006-.
- Fellow of the American Physical Society, 2004.
- Fellow of the American Society of Mechanical Engineers, 2003.
- Associate Editor of Journal of Computational Physics, 2005.

Publications

1. X. Wan and G.E. Karniadakis, "Error control in multi-element generalized polynomial chaos method for elliptic problems with random coefficients", Communication in Computational Physics, vol. 5, pp. 793-820, 2009.

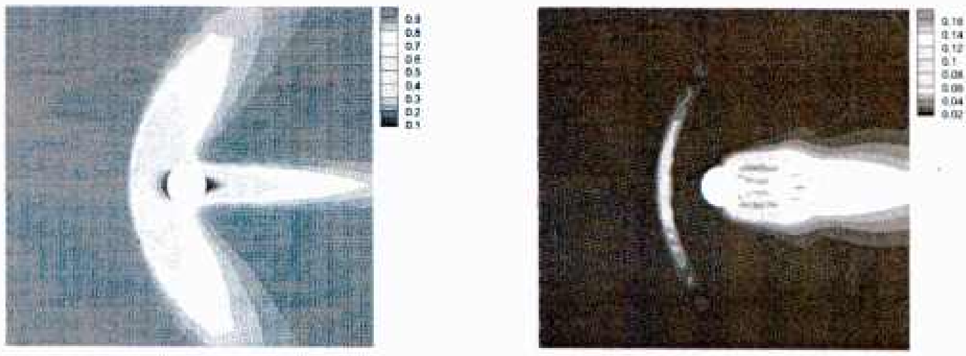
2. X. Wan and G.E. Karniadakis, "Solving elliptic problems with non-Gaussian spatially-dependent random coefficients: algorithms, error analysis and applications", Comput. Methods Appl. Mech. Engr., in press, 2009.

3. J. Foo, X. Wan and G.E. Karniadakis, "The multi-element probabilistic collocation method: error analysis and simulation", J. Comp. Phys., vol. 227, pp. 9572-9595, 2008.

4. D. Venturi, X. Wan and G.E. Karniadakis, "Stochastic low dimensional modeling of random laminar wake past a circular cylinder", Journal of Fluid Mechanics, vol. 606, pp. 339-367, 2008.

5. G. Lin, C.-H. Su and G.E. Karniadakis, "Stochastic modeling of random roughness in shock scattering problems: Theory and simulations", Computer Methods in Applied Mechanics and Engineering, vol. 197, pp. 3420-3434, 2008.

6. G. Lin, C.-H. Su and G.E. Karniadakis, "Random roughness enhances lift in supersonic flow", Phys. Rev. Lett., vol. 99, (10), 104501, 2007.



(a) (b)

Figure 4: (a) Mean and (b) standard deviation of streamwise velocity contours for Re_i described as a random process with correlation length $A = 1$ and $\epsilon = 0.5$.

7. G. Lin and G.E. Karniadakis, "Stochastic simulations and sensitivity analysis of plasma Flow", Paper 2008-1073, 46th AIAA Aerospace Sciences Meeting and Exhibit 7-10 January 2008, Reno, Nevada, also to appear in I. J. Num. Meth. Eng., 2009.

8. G. Lin, X. Wan, C.-H. Su and G.E. Karniadakis, "Stochastic fluid mechanics", IEEE Computing in Science and Engineering (CiSE), vol. 9, pp. 21-29, 2007.

9. X. Wan and G.E. Karniadakis, "Adaptive numerical solutions of stochastic differential equations", Computer Mathematics & its Applications, pp. 561-573, 2006.

Interactions/Transitions

The main interactions have been with:

(1) Dr. Banaszuk, Andrzej, United Technology Research Center, UTRC, BanaszA@utrc.utc.com and

(2) Dr. Philip Beran, Principal Research Aerospace Engineer, WPAFB, OH 45433, Phone 937-255-6645.

Also, the PI has co-edited with Prof. James Glimm (Stonybrook) a special issue of the Journal of Computational Physics focused on uncertainty quantification. He had also interactions with Drs. Robert Canfield and R. Grandhi (Air Force Institute of Technology), and Prof. A. Monti (University of South Carolina) on issues related to uncertainty quantification, and stochastic simulations and specifically on the generalized Polynomial Chaos method.